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NUMERICAL METHODS FOR STIFF AND QUADRATIC  
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(FINAL REPORT)

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## LIST OF CONTENTS

## I. STABILITY AND CONTRACTIVITY OF MULTISTEP AND ONE-LEG METHODS

- A. Background**
- B. Contractivity Results**
  - 1.  $A_0$ - and  $A(\alpha)$ -contractivity results
  - 2.  $A$ -contractivity for two-step methods
  - 3.  $A$ -contractivity for formulas of arbitrary length
- C. Nonlinear Stability Results Based on Contractivity**
- D. Special Methods and Aspects of Implementation**
  - 1. Special contractive methods
  - 2. Formula selection strategy for global error control
  - 3. Multistep and one-leg methods for mixed differential-algebraic systems

## II. NONLINEAR STABILITY OF HIGH ORDER METHODS FOR STIFF EQUATIONS

- A. Background**
- B. Methods and Multipliers**
- C. Nonlinearities and Multipliers**
- D. Boundedness and Stability results**
  - 1. Error bounds**
  - 2. Boundedness**
  - 3. Convergence**
  - 4. Input-output stability**

### III. EXTENDED JOSEPHSON JUNCTIONS AND INTERFEROMETERS

- A. Background**
- B. Extended Junctions**
  - 1. Perturbation results**
  - 2. Existence, uniqueness, and stability results**
  - 3. Quasi-periodic solutions**
- C. Interferometers**
  - 1. Existence of solutions**
  - 2. Numerical perturbation methods for interferometers**
  - 3. Numerical results**

#### IV. SPECIAL METHODS FOR QUADRATIC SYSTEMS OF DIFFERENTIAL EQUATIONS

## V. CUMULATIVE LIST OF PUBLICATIONS



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# I. STABILITY AND CONTRACTIVITY OF MULTISTEP AND ONE-LEG METHODS

## A. Background

With a linear multistep formula,

$$\sum_{j=0}^k \alpha_j x_{n+j} - h \sum_{j=0}^k \beta_j \dot{x}_{n+j} = 0, \quad (1)$$

normalized by

$$\sum_{j=0}^k \beta_j = 1, \quad (2)$$

we can associate two integration methods for systems of ordinary differential equations

$$\dot{x} = f(t, x) \quad (3)$$

namely the linear multistep (MS) method

$$\sum_{j=0}^k \alpha_j x_{n+j} - h \sum_{j=0}^k \beta_j f(t_{n+j}, x_{n+j}) = 0 \quad (4)$$

and its one-leg (OL) "twin"

$$\sum_{j=0}^k \alpha_j x_{n+j} - h f\left(\sum_{j=0}^k \beta_j t_{n+j}, \sum_{j=0}^k \beta_j x_{n+j}\right) = 0. \quad (5)$$

The formula (1) is said to be stable at  $q = h\lambda$  if all solutions  $\{x_n\}$  of the difference equation, generated by applying (1) to the test equation

$$\dot{x} = \lambda x, \quad \lambda \text{ complex, constant}, \quad (6)$$

(for which the MS- and OL-methods are identical) remain bounded for a given  $h > 0$  as

$n \rightarrow \infty$ . This is the case iff the characteristic polynomial

$$\chi(\zeta) = \rho(\zeta) - q\sigma(\zeta) \quad (7)$$

satisfies the "root condition" (i.e., all roots  $\zeta_i$  of  $\chi(\zeta)$ ,  $i = 1, \dots, k$ , satisfy  $|\zeta_i| \leq 1$  and  $|\zeta_i| = 1 \Rightarrow \zeta_i$  is simple). Here

$$\rho(\zeta) = \sum_{j=0}^k \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^k \beta_j \zeta^j. \quad (8)$$

The stability region  $S$  is the set of all  $q$  at which the formula is stable. The formula is said to be  $A^-$ ,  $A_0^-$ , and  $A_\infty^-$ -stable, if  $\mathcal{C}_- := \{q | \operatorname{Re} q \leq 0\}$ ,  $\mathcal{R}_- := \{q | q \leq 0\}$ , or  $\{q = \infty\}$  are contained in  $S$ , respectively.

The formula (1) is said to be contractive [8] at  $q$  with respect to a given norm  $\|\cdot\|$  if  $\|X_{n-1}\| \geq \|X_n\|$  for all  $n \geq k$ , where  $X_n := (x_{n-k+1}, x_{n-k+2}, \dots, x_n)$ . The contractivity region  $K$  (with respect to  $\|\cdot\|$ ) is the set of all  $q$  at which the formula is contractive. The formula is said to be  $A^-$ ,  $A_0^-$ , or  $A_\infty^-$ -contractive, if  $\mathcal{C}_-$ ,  $\mathcal{R}_-$ , or  $\{q = \infty\}$  are contained in  $K$ , respectively. Clearly, contractivity at  $q$ ,  $A$ -contractivity, etc., imply the corresponding stability properties, since  $K \subseteq S$ . Contractivity is a useful tool for obtaining stability results for nonlinear problems or equations with variable coefficients, and for variable integration steps, as well as for identifying novel, very robust integration formulas. A survey of contractivity results is given in [17].

## B. Contractivity Results

### 1. $A_0^-$ and $A(\alpha)$ -contractivity results.

The formula (1) is  $A_\infty^-$ -contractive with respect to the  $\ell_\infty$ -norm iff  $\gamma := \beta_k - \sum_{j=0}^{k-1} |\beta_j| \geq 0$ . Subject to the normalization (2), one has  $\gamma \leq 1$ . We proved [8] that for any  $p$  there exist formulas of order  $p$  which are  $A(\alpha)$ -contractive with respect to the max norm for any  $\alpha$  smaller than, but arbitrarily close to  $\pi/2$  and whose

measure of  $A_\infty$ -contractivity,  $\gamma$ , is arbitrarily close to unity. (Note that since  $A$ -contractivity implies  $A$ -stability, this result for  $p \geq 3$  is as strong as it can be). In general, however, the length  $k$  of these methods grows approximately like  $3p$ .

We derived [14] the two-parameter class of all two-step ( $k = 2$ ) second-order ( $p = 2$ ) formulas which are  $A_0$ -contractive w.r. to the maximum norm  $\|\cdot\|_\infty$  for arbitrary step ratios  $r = r_n = h_n/h_{n-1}$ . This generalized the corresponding results for uniform steps given in [8]. For the test problem  $\dot{x} = \lambda(t)x$  with arbitrary  $\lambda(t) \leq 0$ , the OL-implementation of any variable-step  $A_0$ -contractive formula provides an  $A_0$ -stable method for arbitrary step sequences  $\{h_n\}$ .

## 2. $A$ -contractivity for two-step methods

We proved [8] that a MS-formula which is  $A_0$ -contractive with respect to the max norm is  $A$ -contractive if and only if it satisfies the constraint

$$\sum_{j=0}^{k-1} [(\alpha_j^2 + \beta_j^2 \eta) / (\alpha_k^2 + \beta_k^2 \eta)]^{1/2} \leq 1, \quad 0 \leq \eta \leq +\infty. \quad (9)$$

In general, (9) is not easy to analyze but for the 2-parameter family of all MS-formulas with  $p \geq 2$ , defined by

$$a_0 = \frac{1}{2}(-1 + b_1), \quad \alpha_1 = -b_1, \quad \alpha_2 = \frac{1}{2}(1 + b_1), \quad (10)$$

$$\beta_0 = \frac{1}{4}(1 + b_0 - b_1), \quad \beta_1 = \frac{1}{2}(1 - b_0), \quad \beta_2 = \frac{1}{4}(1 + b_0 + b_1),$$

the condition (9) is satisfied iff [8]

$$b_0 = 1 - b_1^2, \quad 0 \leq b_1 \leq 1. \quad (11)$$

As stated in [8], the special formula

$$-\frac{1}{6}x_n - \frac{4}{6}x_{n+1} + \frac{5}{6}x_{n+2} - h\left(\frac{2}{9}\dot{x}_n + \frac{2}{9}\dot{x}_{n+1} + \frac{5}{9}\dot{x}_{n+2}\right) = 0 \quad (12)$$

minimizes a bound for the global truncation error derived in [9], over all A-contractive  $p = k = 2$ -formulas. (See subsection I. D.1 hereafter.)

We generalized the one parameter class of all  $p = k = 2$ -formulas which are A-contractive w.r. to  $\|\cdot\|_\infty$  to arbitrary step ratios  $r = r_n = h_n/h_{n-1}$  [14]. It is defined by

$$\begin{aligned} \alpha_{0,n} &= -\frac{r^2}{1+r}(1-v), & \beta_{0,n} &= \frac{r}{1+r} + \frac{r(r-2)}{2(1+r)}v - \frac{r^2}{2(1+r)}v^2, \\ \alpha_{1,n} &= -[1-r(1-v)], & \beta_{1,n} &= \frac{1-r}{2}v + \frac{r}{2}v^2, \\ \alpha_{2,n} &= 1 - \frac{r}{1+r}(1-v), & \beta_{2,n} &= \frac{1}{1+r} + \frac{2r-1}{2(1+r)}v - \frac{r}{2(1+r)}v^2, \end{aligned} \quad (13)$$

where the formula is to be read as  $\sum_{j=0}^2 \alpha_{j,n} x_{n-2+j} - h_n \sum_{j=0}^2 \beta_{j,n} \dot{x}_{n-2+j} = 0$ , and the parameter  $v$  satisfies

$$\frac{r-1}{r} \leq v \leq 1. \quad (14)$$

We proved [14] that any formula with  $p = k = 2$  is A-contractive w.r. to  $\|\cdot\|_\infty$  iff it is G-stable, i.e., A-contractive w.r. to some G-norm (a norm associated with a positive definite quadratic vector form). For any given A-contractive  $p = k = 2$  formula with  $r = 1$  (uniform steps), specified by a parameter value  $v = v_1$ ,  $0 \leq v_1 \leq 1$ , A-contractive extensions to non-uniform steps ( $r \neq 1$ ) can be defined in such a way as to keep the G-norm fixed w.r. to  $n$  [14]. If this is done then, for an arbitrary



step sequence  $\{h_n\}$ , G-stability is assured for any dissipative (monotone negative) nonlinear system.

We proved [13,14] that, except for borderline cases, the A-stable and A-contractive  $p = k = 2$ -formulas can be identified by a local analysis near  $q = 0$  and for small non-uniformities of the grid. More specifically, for uniform and nonuniform grids, stability in any arbitrarily small left half-neighborhood of  $q = 0$  is, roughly speaking equivalent to A-stability (for the latter in the formal algebraic sense that  $\rho(\zeta) - q\sigma(\zeta)$  satisfy the "root condition" (r.c.) for all  $q, \operatorname{Re} q \leq 0$ ). Furthermore, requiring that the r.c. remain satisfied for  $r = r_n = 1 + \varepsilon$  under arbitrary perturbations around  $\varepsilon = 0$  singles out all A-contractive methods with uniform steps.

### 3. A-contractivity for formulas of arbitrary length

In [16] we generalized the derivation of the variable step A-contractive second-order-formulas mentioned above from  $k = 2$  to arbitrary length. First of all, the formula (1) is  $A_0$ -contractive iff [8]

$$\begin{aligned} -\alpha_j &\geq 0, \quad j = 0, \dots, k-1, \\ \beta_k - \sum_{j=0}^{k-1} |\beta_j| &\geq 0, \end{aligned} \tag{15}$$

and  $\alpha_k > 0$  (the latter follows from the first of relations (15) by consistency and the assumption that  $\alpha_k \neq 0$ ). Subject to (15) and for  $\alpha_j \neq 0$ , the formula is A-contractive iff [8].

$$F(\eta) = \sum_{j=0}^k \alpha_k [1 + (\beta_j^2 \eta / \alpha_j^2)]^{1/2} \geq 0, \quad \eta \geq 0 \tag{16}$$

where  $q = iy$ ,  $y$  is real and  $\eta = y^2$ . By consistency,  $F(\eta) = \frac{1}{2}\eta F + O(\eta^2)$  for  $\eta \rightarrow 0$ ,

and

$$F := \sum_{j=0}^k (\beta_j^2 / \alpha_j) \geq 0 \quad (17)$$

is thus necessary for (16) to hold. We proved a) that the only  $p = 2$ -formulas satisfying (17) are defined by

$$\beta_j = (\theta_{k-j} - \frac{1}{2} A_2)(-\alpha_j), \quad j = 0, 1, \dots, k \quad (18)$$

where  $\theta_j = \theta_{j,n} := (t_n - t_{n-j})/h_n$  and  $A_2 := -\sum_{j=0}^k \theta_{k-j}^2 \alpha_j$ ; and b) that (17) is also sufficient for (16) to hold and thus (15) and (17) together define the set of all A-contractive formulas. Consistency requires that

$$\begin{aligned} \alpha_k &= 1 - \sum_{j=0}^{k-2} (\theta_{k-j} - 1)(-\alpha_j), \\ \alpha_{k-1} &= - \left[ 1 - \sum_{j=0}^{k-2} \theta_{k-j}(-\alpha_j) \right], \end{aligned} \quad (19)$$

and thus the A-contractive formulas are in one-to-one correspondence with the points of a simplex, in the space spanned by the  $(k-1)$  free parameters  $\alpha_0, \dots, \alpha_{k-1}$ , whose vertices are the origin and  $\{-\alpha_j = 1/\theta_{k-j}, \alpha_i = 0, i \neq j; j = 0, \dots, k-2\}$ . These vertices represent respectively, as degenerate  $j$ -step formulas, the Trapezoidal Rules with step lengths  $t_n - t_{n-j}, j = 0, \dots, k$ .

To illustrate the significance of the above theorem we remark that stability can be guaranteed for *arbitrary* step sequences if at each integration step *any one* of the A-contractive OL-methods is applied to  $\dot{x} = \lambda(x)x$  with *any*  $\lambda(t)$ ,  $\text{Re } \lambda(t) \leq 0$ . This behavior is in marked contrast to that of the popular two-step second-order backward differentiation formula which can be destabilized by certain combinations of variable steps and coefficients, as exemplified hereafter:

For exponentially varying grids, i.e.  $h_n = h_1 r^{n-1}$ ,  $n = 1, 2, \dots, r \neq 1$ , and for  $\lambda(t) = r h_1 \lambda_1 [h + (r-1)t]^{-1}$ , the formula and the difference equation generated by applying a one-leg method to  $\dot{x} = \lambda(t)x$  have constant coefficients and stability can be analyzed algebraically [14]. For this problem with increasing steps ( $r > 1$ ), the backward differentiation formula (BDF) with  $p = k = 2$  loses A-stability [12 - 14]. For  $r < 1$  the BDF is A-stable but when applied to purely oscillatory problems ( $\text{Re } \lambda_1 = 0$ ) it is too strongly damped. The A-contractive  $p = k = 2$  one-leg methods, on the other hand, are A-stable for this problem for any  $r$  and accurately reflect the constant amplitude of purely oscillatory solutions [12,13].

As a generalization of the corresponding result for  $k = 2$  mentioned above we proved in [16], for arbitrary  $k$ , that the A-contractive formulas for uniform steps can also be derived without invoking the contractivity concept, but instead by analyzing a necessary algebraic condition for A-stability for mildly non-uniform grids. The condition in question is

$$|\zeta_1(q)| \leq 1 \quad (20)$$

for  $q = iy$ ,  $y$  real,  $|y|$  sufficiently small, where  $\zeta_1(q)$  denotes the principle root of the characteristic polynomial  $\Sigma(\alpha_j - q\beta_j)\zeta^j$  (the one defined by  $\zeta_1(0) = 1$ ). The coefficients  $\alpha_j$ ,  $\beta_j$  are associated with a mildly variable grid, i.e., one for which  $\theta_j = j + \varepsilon_j$ ,  $|\varepsilon_j| \ll 1$ . By a perturbation analysis with respect to the  $\varepsilon_j$  one can show that the only  $p = 2$ -formulas for constant steps ( $\varepsilon_j = 0$ ) which can smoothly be extended to arbitrary  $\varepsilon_j$ ,  $|\varepsilon_j|$  small, in such a way that (20) remains satisfied to first-order in the  $\varepsilon_j$  are the A-contractive formulas.

### C. Nonlinear Stability Results Based on Contractivity

In [9] we gave a boundedness result for solutions, generated by an A(0)-

contractive formula, of a system of the form

$$\dot{x} = A(t, x)x + d(t, x), \quad (21)$$

where  $A = (a_{ij}(t, x))$  is a real matrix with  $a_{ii} < 0$  and a certain amount of diagonal dominance and  $d(t, x)$  is bounded. Subsequently, in [13], we gave a sharper result and a more transparent proof. Specifically, we showed that if we apply to (21) a one-leg method which is both contractive at  $q = 0$  and (strictly) contractive at  $q = \infty$  with respect to the  $l_\infty$ -norm (i.e. if  $a_j \leq 0$ ,  $j = 0, \dots, k-1$ ,  $\alpha_k > 0$  and  $\gamma = \beta_k - \sum_{j=0}^{k-1} |\beta_j| > 0$ , respectively) then we have input-output stability in the  $l_\infty$ -norm provided  $B = (b_{ij})$  is a M-matrix; here  $b_{ii} = -a_{ii}\gamma$  and  $b_{ij} = -(\sum_{j=0}^k |\beta_j| \sup_{t, x} |a_{ij}(t, x)|)$ . The two results mentioned in this paragraph are the only nonlinear stability results we are aware of which are based on contractivity analysis and which do not assume monotonicity of the nonlinear system but rather a type of diagonal dominance of  $A$ . Note that this result is of a novel type in the sense that it is valid for all  $h > 0$  without requiring A-stability. Earlier nonlinear results based on stability and relevant for stiff problems either required A-stability (and thus apply only to methods with  $p \leq 2$ ) or they were valid only for sufficiently large  $h$ .

#### D. Special Methods and Aspects of Implementation

##### 1. Special contractive methods.

A special  $A_0$ -contractive formula with  $p = k = 2$  was selected in [9] which minimizes a bounded of the global error produced by applying any  $A(0)$ -contractive OL-method to the model problem  $\dot{x} = \lambda(t)x$ ,  $\lambda(t) \leq -a < 0$ ,  $t \geq 0$ . The formula in question,

$$x_{n+2} - x_{n+1} - h \left( \frac{3}{4} \dot{x}_{n+2} + \frac{1}{4} \dot{x}_n \right) = 0, \quad (22)$$

is of Adams type. We proved [9] that the one-leg implementation of this method remains  $A_0$ -contractive (and thus  $A_0$ -stable) for any variable step sequence whatsoever as well as for  $t$ -dependent  $\lambda$ . For  $r = r_n = h_n/h_{n-1}$ , its coefficients are defined by  $\alpha_{0,n} \equiv 0$ ,  $\alpha_{1,n} \equiv -1$ ,  $\alpha_{2,n} \equiv 1$ ,  $\beta_{0,n} = r/(2+2r)$ ,  $\beta_{1,n} \equiv 0$ , and  $\beta_{2,n} = (2+r)/2+2r$ . By minimizing the same objective function over the class of all A-contractive  $p = k = 2$ -formulas with uniform steps we found [8,14] the special A-contractive formula given by (12) which is associated with  $v = v_1 = \frac{2}{3}$ . This formula was generalized [14] by extending its minimality property to the variable step case. For arbitrary  $r$  it is defined by  $v = 2r/(2r+1)$  and has coefficients

$$\begin{aligned} \alpha_0 &= -\frac{r^2}{(1+r)(1+2r)}, \quad \beta_0 = \frac{r(1+r)}{(1+2r)^2} \\ \alpha_1 &= -\frac{1+r}{1+2r}, \quad \beta_1 = \beta_0 \\ \alpha_2 &= \frac{1+2r+2r^2}{(1+r)(1+2r)}, \quad \beta_2 = \frac{1+2r+2r^2}{(1+2r)^2}. \end{aligned} \quad (23)$$

## 2. Formula selection strategy for global error control.

Given any sequence of steps  $\{h_n\}$  whose ratios  $r_n = h_n/h_{n-1}$  are bounded away from zero and infinity, and any  $\lambda(t)$  satisfying  $\operatorname{Re} \lambda(t) \leq -a, a > 0$ , we derived [13] a simple strategy (local in  $t$ ) for selecting a sequence of A-contractive one-leg methods with  $p = k = 2$  in such a way as to minimize an upper bound of the global truncation error produced by integrating  $\dot{x} = \lambda(t)x$ .

### 3. Multistep and one-leg methods for mixed differential algebraic systems

Systems of the form

$$\begin{aligned} F(t, \dot{x}, x, y) &= 0 \\ G(t, x, y) &= 0 \end{aligned} \tag{24}$$

are often encountered in applications. Here  $F$  and  $x$  are vectors of the same dimension and so are  $G$  and  $y$ . In [10] we proposed and analyzed one MS-implementation and two OL-implementations of the formula (1). The particular methods of this type associated with the variable step version of the  $A(\alpha)$ -contractive Adams formula defined by (22) was shown to be second-order accurate, both in the "differentiated variables"  $x$  and in the "state variables"  $y$ . All three implementations were tested numerically on a nonlinear diode circuit problem. The numerical results were in very good agreement with the theoretical findings.

## II. NONLINEAR STABILITY OF HIGH ORDER METHODS FOR STIFF EQUATIONS

### A. Background

High-order linear multistep methods (LMM) have computational advantages in the numerical integration of stiff problems whose solutions are sufficiently smooth. One usually assumes in such situations that the spectrum of the Jacobian of the nonlinearity stays within a sectorial set and, correspondingly, one uses high-order  $A(\alpha)$ -stable schemes. The techniques used in studying the nonlinear stability of low-order methods, e.g., A- and G-contractivity are not applicable to the high-order ones and a corresponding nonlinear stability theory has been lacking. We have introduced [15] a new technique to investigate the behavior of the numerical errors in high-order LMM when applied to parabolic-like nonlinear problems. We consider the global error equation

$$\gamma * e_n + h[f(x_n + e_n) - f(x_n)] = h q_n, \quad (25)$$

where  $\gamma$  is the  $\ell_1$ -sequence defined by  $\rho\sigma^{-1}(\zeta) = \sum_j \gamma_j \zeta^{-j}$ ,  $x_n$  is the approximate solution,  $q_n$  is the local error,  $e_n$  the global error,  $h$  the uniform time step,  $f(\cdot)$  the nonlinearity in the stiff differential system and  $*$  denotes convolution. Instead of scalar multiplication of (25) with  $e_n$ , we multiply by  $\mu * e_n$ , where  $\mu$  is an appropriately chosen sequence called the "multiplier" and is defined hereafter. This procedure yields two "energy-like" error terms, namely a quadratic term describing the interaction between the multiplier and the method, and a more general nonlinear term combining the problem with the multiplier. To control the global error, both terms have to be positive and our stability theory finds conditions for such positivity. The results naturally subdivide to cover three areas: the relationship between the multistep

method and the multiplier, the interaction of the nonlinearity with the multiplier, and finally boundedness, stability, and convergence results.

First, a definition is given for multipliers: Let  $(\rho, \sigma)$  be the usual polynomials defining a multistep method; then

Definition: A sequence  $\mu = (\mu_0, \mu_1, \dots)$  is a rational multiplier for the method  $(\rho, \sigma)$  if 1) its  $z$ -transform is rational, 2) its Fourier transform  $\hat{\mu}(\tau) = \sum \mu_n e^{-in\tau}$  has positive real part, and 3) there exists a  $\delta > 0$  such that

$$\operatorname{Re} \left\{ \overline{\hat{\mu}(\tau)} \frac{\delta}{\sigma}(e^{i\tau}) \right\} \geq \delta \tau^2, |\tau| \leq \pi. \quad (26)$$

All results mentioned in subsections II B, C, and D hereafter are proved and described in detail in [15].

## B. Methods and Multipliers

Recall (a) that the stability region  $S$  of a method  $(\rho, \sigma)$  is the set of all complex  $q$ 's such that the difference equation  $\sum_{j=0}^k (\alpha_j - q\beta_j)x_{n-k+j} = 0$  has only bounded solutions, and (b) a method is said to be  $A(\alpha)$ -stable if  $\{re^{i\phi} \mid r \geq 0, |\pi - \phi| \leq \alpha\} \subset S$ .

1) It was shown that linear stability theory of  $A(\alpha)$ -stable methods is derivable in a simple, elegant way by the multiplier technique. This is mainly a consequence of the following existence theorem:

Theorem 1: If a method  $(\rho, \sigma)$  is  $A(\beta)$ -stable, then, for any  $0 < \alpha < \beta$ , there exists a multiplier of finite support,  $\mu = \{\mu_j\}_0^M$ , for  $(\rho, \sigma)$  such that

$$|\arg \hat{\mu}(\tau)| < \frac{\pi}{2} - \alpha. \quad (27)$$



Since it is easy to see that (27) implies  $A(\alpha)$ -stability, Theorem 1 may be interpreted as saying that the linear stability of an  $A(\alpha)$ -stable method can be "seen" through the multiplier.

2) A quantitative "uncertainty principle" was derived showing the incompatibility of extreme stability and accuracy of a method. The error in a method may be measured by the size of the Fourier transform of the associated Peano kernel  $K$ , and its stability by  $\eta^{-1}$  where  $(1, -\eta, 0, \dots)$  is the special Popov multiplier associated with the method. In this case one has

Theorem 2: For every  $k$ , there exists  $C_k > 0$  such that, if  $\{1, -\eta\}$  is a multiplier for the  $k$ -step method  $(\rho, \sigma)$  then, as  $\eta \rightarrow 0$ ,

$$\|\hat{K}\| \geq C_k \eta^{2-p},$$

showing the blow-up of the error if  $p > 2$  and  $\eta \rightarrow 0$ .

3) A graphical method was devised for determining whether a method possesses a multiplier of the Popov type. This type of multiplier is especially convenient for proving nonlinear stability results. The method was applied to exhibit the stability of the BDF of orders 2-5.

### C. Nonlinearities and Multipliers

Positivity results for the "energy-like" quantities of the form

$$\sum_N \langle \mu \circ v_n, F_n \rangle \geq 0, \quad (28)$$

where  $F_n = f(nh, v_n)$  or  $F_n = f(nh, x(nh) + v_n) - f(nh, x(nh))$  and where  $x(nh)$  denotes the exact solution of the stiff system and  $\langle, \rangle$  the scalar product, are necessary for proving nonlinear stability of the LMM when applied to  $\dot{x} = f(t, x)$ . We give

examples of such results which may be thought of as "Generalized Correlation Inequalities" and which are of general interest.

Lemma 1:

1) Let  $\phi$  be convex, non-negative and  $\phi(0) = 0$ . Let  $\mu_j \leq 0$  for  $j \geq 1$  and let  $P$  be the sequence of partial sums of  $\{\mu\}$ ; then

$$\sum_{n=1}^N \langle \mu \circ v_n, \text{grad } \phi_n \rangle \geq (P\mu \circ \phi)_N.$$

2) The nonlinearity is said to be gradient-like, or more precisely,  $\sigma$ -angle-bounded, if

$$\langle f(x) - f(y), y - z \rangle \leq \sigma \langle f(x) - f(z), x - z \rangle. \quad (29)$$

An example are the 3-monotone functions satisfying

$$\sum_{i=1}^3 \langle x_i - x_{i-1}, f(x_i) \rangle \geq 0, x_0 = x_3.$$

In this case, we have

Lemma 2: If  $f$  is  $\sigma$ -angle-bounded,  $f(0) = 0$  and  $\mu_j \leq 0$  for  $j \geq 1$ , then

$$\sum \langle \mu \circ v_n, f_n \rangle \geq [\mu_0 - (1 + \sigma) \sum_1^{\infty} |\mu_j|] \sum \langle v_n, f_n \rangle. \quad (30)$$

3) For proving convergence results for LMM, we employ the following useful inequality:

Lemma 3: Let  $F(u, v) = f(u, x_n + v) - f(u, x_n)$  then

$$\sum \langle \mu \circ v_n, F_n \rangle \geq \mu_0 - \left( \sum_1^{\infty} |\mu_j| \right) K_1 \left( \frac{1 + K_2}{2} \right) \sum \langle v_n, F_n \rangle.$$

where  $K_1, K_2$  measure the asymmetry and time-variation of  $f$ , respectively; i.e.,

$$\langle u, J(t)v \rangle \leq \frac{K_1}{2} [\langle u, Ju \rangle + \langle v, Jv \rangle], \quad (31)$$

$$\langle u, J(t, x)u \rangle \leq K_2 \langle u, J(s, y)u \rangle, \quad (32)$$

where  $J$  = Jacobian of  $f$ .

4) Positivity results are also obtained for general, not necessarily monotone, functions if they are nearly linear, as in the following lemma.

Lemma 4: Let  $F(u, v) = Hv + Hg(u, v)$  where  $H = H^T \geq 0$  and assume that

$$\langle g(v), Hg(v) \rangle \leq L \langle v, Hv \rangle.$$

Then

$$\sum \langle \mu^* v_n, F_n \rangle \geq (m_0 - L \|\hat{\mu}\|_\infty) \sum \langle v_n, Hv_n \rangle,$$

where  $m_0 = \min \operatorname{Re} \hat{\mu}$ .

#### D. Boundedness and Stability Results

Various boundedness and stability results for the numerical solution of difference equations, arising when  $A(\alpha)$ -stable methods are applied to nonlinear systems, were obtained when the nonlinearity and the multiplier "match" (in the sense that the inequality (28) holds, as is the case for example, in Lemmas 1-4 above).

##### 1. Error bounds.

We consider the difference equation

$$\rho(E)x_n + h\sigma(E)F_n = hp_{n+k} \quad (33)$$

where  $p_n$  denotes the local error (or a forcing term),  $x_n$  the global error (or the computed solution), and  $F_n$  the global error in  $f$  (or the nonlinearity itself, respectively). Then if  $F$  satisfies (28), we have the basic boundedness result that, for some  $C$ ,

$$|x_n| \leq C \left\{ \max_{0 \leq j \leq k} |x_j| + h|F_j| + h \sum_{j=k}^n |p_j| \right\}. \quad (34)$$

Equation (34) shows that global errors are, under such conditions, controlled by local errors.

## 2. Boundedness.

We have shown that a) if the perturbations in (33) are summable, then (28) holds; b) if  $f(0) = 0$  and  $f$  is maximally monotone (though, possibly, discontinuous) then, as  $n \rightarrow \infty$ , every solution of the difference equation tends to a unique value of  $f^{-1}(0)$ . Hence, if  $f^{-1}(0) = 0$  as is usually the case, all solutions tend to zero as  $t \rightarrow \infty$ .

## 3. Convergence.

It was shown that if a method of order  $p$  has a multiplier compensating for the asymmetry of the problem, in the sense that  $K_1 \sum_{j=1}^{\infty} |\mu_j| < \mu_0$  [see equation (31)], then for small  $h$  and  $nh \leq T$  one has

$$|\text{global numerical error}| \leq CTh^p.$$

## 4. Input-output stability.

We have also proved  $\ell_2$ - and  $\ell_\infty$ -input - output stability of (33) under slightly technical assumptions.

### III. EXTENDED JOSEPHSON JUNCTIONS AND INTERFEROMETERS

#### A. Background

The Josephson phase equation, describing an extended junction, is

$$\Lambda \phi \equiv \frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} - \frac{\partial \phi}{\partial t} = k \sin \phi \quad (35)$$

where  $\phi$  is the phase and  $\sigma$ ,  $k$  are, resp., related to the normal and Josephson tunneling currents. One seeks solutions  $\phi$  such that  $\frac{\partial \phi}{\partial t}$  is periodic of a certain period  $\frac{2\pi}{\omega}$  where  $\omega$  is equal to the d.c. voltage. If these solutions are non-static they are called running solutions. The boundary conditions on  $\phi$  depend on the manner in which the junction is driven and they read

$$\phi|_{x=0} = \omega t, \quad \frac{\partial \phi}{\partial x}|_{x=\pi} = -H_e \quad (36)$$

in the voltage-driven case, or

$$\frac{\partial \phi}{\partial x}|_{x=0} = -(H_e + I_e), \quad \frac{\partial \phi}{\partial x}|_{x=\pi} = -H_e \quad (37)$$

in the current-driven case. Here  $H_e$ ,  $I_e$ ,  $\omega$  are the external magnetic field, total current and d.c. voltage, respectively.

A "point" junction is one that is "small enough" for the term  $\partial^2 \phi / \partial x^2$  in (35) to be negligible; in this case, the phase equation becomes an ordinary differential equation. Interferometers consist of a given number  $n$  of point junctions connected in various manners and "loaded" by currents. We have been interested in studying the properties, especially the I-V characteristics, of the extended junction as well as the

symmetric, two-junction current driven interferometer, whose equations are

$$\begin{aligned}\beta\ddot{\phi}_1 + \alpha\dot{\phi}_1 + \sin \phi_1 + \lambda^{-1}(\phi_1 - \phi_2) &= I/2 + I_c \\ \beta\ddot{\phi}_2 + \alpha\dot{\phi}_2 + \sin \phi_2 + \lambda^{-1}(\phi_2 - \phi_1) &= I/2 + I_c;\end{aligned}\tag{38}$$

here  $\lambda$  is proportional to the inductance,  $I_c$  is a control-current and  $\phi = \omega t +$  periodic of period  $2\pi/\omega$ , where  $\omega$  is proportional to the voltage.

## B. Extended Junctions

### 1. Perturbation results.

The running solutions and I-V characteristic of an extended Josephson junction in a state near the ohmic regime were calculated by a perturbation method. Both the voltage-driven and current-driven cases were considered and the convergence of the perturbation procedure was proved. An integral representation of the first correction, in the I-V curve, to the ohmic regime-as well as its dependence on the external magnetic field-was given and evaluated numerically for various values of the junction parameters. The details of these results were given in [6].

### 2. Existence, uniqueness, and stability results.

If one writes  $\phi = \phi_0 + \psi$ , where

$$\phi_0 = \omega t - kx + \rho x^2$$

satisfies the formal limit equation  $\Lambda\phi_0 = 0$  as  $\kappa \rightarrow 0$ , and where  $k = \sigma\omega + H_c$ ,  $\rho = \sigma\omega/2$ , and  $\psi$  is periodic, then in the voltage driven case  $\psi$  satisfies

$$\begin{aligned}\Lambda\psi &= \kappa \sin(\phi_0 + \psi), \\ \psi|_{x=0} &= \frac{\partial\psi}{\partial x}|_{x=\pi} = 0.\end{aligned}\tag{39}$$

The following results were proved in this case:

a) For any  $\sigma \neq 0$  there exist  $(2\pi/\omega)$ -periodic solutions of the problem (39).

Hence, for  $\sigma \neq 0$ , there exist (possibly multiply branched I-V characteristics for the Josephson junction.

b) For moderate amounts of dissipation relative to the strength of the nonlinearity (i.e., moderately large values of  $\sigma$  relative to  $\kappa$ ), the periodic solution of (39) is unique and globally asymptotically stable. Hence solutions with arbitrary initial data tend, exponentially in  $t$ , to  $\phi = \phi_0 + \psi$  with  $\psi$  periodic. For example, if  $\kappa = \frac{1}{8}$  (corresponding to  $L/\lambda_J \sim .9$ ) then  $\sigma \geq 9/16$  is sufficient for uniqueness; similarly, with  $\kappa = 1/4\pi^2$  (corresponding to  $L/\lambda_J = \frac{1}{2}$ ) uniqueness is assured for  $\sigma \geq .06$ .

The existence theorem a) above was also extended to the current-driven junction where the period  $\omega$  is also unknown.

### 3. Quasi-periodic solutions.

We studied the behavior of the extended junction, described by equation (35), when it is driven by an oscillating voltage source. More specifically, we replaced the first of the boundary conditions (36) by the condition

$$\dot{\phi}|_{x=0} = p(t) \quad (40)$$

where  $p(t)$  is a quasi-periodic function of time with arbitrary fundamental frequencies  $\omega_0, \omega_1, \dots, \omega_n$ . Such problems occur if the junction is used as a detection device. Using some delicate perturbation and estimation arguments, we proved that for  $\sigma > 0$  the phase equation has a quasi-periodic solution which is unique when  $\kappa$  is small.

## C. Interferometers.

### 1. Existence of solutions

We gave a proof of the existence of running solutions to (38) for arbitrary  $\kappa$ , under the assumption that the dimension of the connection matrix is equal to one. The proof uses a homotopy argument to show that, for  $\omega \neq 0$ ,  $\sigma \neq 0$ , there always exists an *odd* number of solutions.

## 2. Numerical perturbation methods for interferometers

We developed efficient numerical methods for finding solutions to (38) and the associated I-V curves. First, for a given  $I$ , perturbation methods are used to find a phase  $\phi$  and voltage  $\omega$  for small  $\kappa$ . The problem is then formulated as a boundary value problem for the pair  $(\phi, \omega)$  with an extra condition on  $\phi$  - derived from the autonomous character of (38) which "determines"  $\omega$ . Under certain assumptions, we proved that the pair  $(\phi, \omega)$  is isolated and that a Newton-like method converges. The basic numerical procedure is a continuation method which gives the whole I-V curve. The procedure was modified in order to improve flexibility, accuracy and efficiency. Specifically:

a) We employed a two-parameter continuation method to compute the solutions, the two parameters being the voltage and the strength of the nonlinearity. This was very useful for finding different branches of solutions by following different continuous paths.

b) Since the calculation was delicate, we checked its accuracy by three different methods:

- 1) by grid refinement;
- 2) by deriving a consistency relation  $I = I(\psi)$  which the exact solution must satisfy and monitoring the discretization error in this relation; and
- 3) by carrying out linear stability calculations.

(Since the translation invariance of equation (38) implies that at least one Floquet multiplier must be unity, this fact was also used to check the accuracy.)



c) To obtain a complete picture of the interferometer, the basic calculation has to be repeated  $10^4 \sim 10^5$  times and thus must be done quite efficiently. The following are some of the features which enhanced the efficiency of our computation:

1) The unknowns in the linearized equations are numbered in an appropriate way for sparse matrix techniques to become applicable. Since these equations depend strongly on  $\omega$ , and weakly on  $\lambda$ , the computation of " $\lambda-\omega$  grid" was arranged so that the outer-most loop was the  $\omega$ -loop, the next was the  $\lambda$ -loop and the inner-most was the Newton loop.

2) The computation took advantage of the consistency, in  $\lambda$ , of the off-diagonal part of the linearized equations.

3) The starting guess for the Newton-loop was obtained by using a "predictor"; this reduced the number of the Newton-steps needed for convergence.

### 3. Numerical results.

The above numerical study yielded the following:

a) The correct dependence of the resonant current on the two physically important parameters  $\lambda$  and  $\Gamma \equiv \frac{1}{\sqrt{2}} \cdot \frac{\sqrt{\beta\lambda}}{\alpha}$ . Previous approximate calculations and physical analysis gave the dependence of this resonant current on  $\Gamma$  alone. Our calculations showed that these previous results are qualitatively valid only for  $\lambda$  around 0.8-1.0. However, they underestimate the maximum resonant current by about 50 percent for these values of  $\lambda$  and are rather invalid elsewhere.

b) There are subharmonic resonances in the I-V curve which occur around one-third of the resonant frequency (voltage) for small  $\lambda$ , but shift towards one-half of the resonant frequency for  $\lambda \sim 1$ , i.e., in the strongly nonlinear case.

c) At resonance, the two phase functions are opposite in sign and for each function all the Fourier components are negligible except for the fundamental frequen-

cy. However, for small voltage,  $\sim 1$  of resonance, the phase functions have an almost saw-tooth shape with many frequencies present.

d) Two types of bifurcations for the solutions to (38). Near, and a little to the left of the main resonance, bifurcation to another  $(2\pi)\omega$ -periodic solution occurs. Bifurcations to  $(4\pi)\omega$ -periodic solutions occur to the right of the main resonance (for values of  $\lambda \sim 2$ ).

e) The dependence of the amplitude of the subharmonic resonances, as well as the main one, on the strength of the nonlinearity (i.e., on the parameter  $\lambda$  in (38)), was computed. The subharmonics are about 15 percent of the main resonance; they are stable for small nonlinearities ( $\lambda \sim .5$ ) but unstable at  $\lambda \sim 1$ .

f) The I-V characteristic curves were found to be generally multi-valued and to possess many loops (even though most of the loops are either unstable or only meta-stable). Hysteretic behavior is clearly evident.

g) Negative resistance portions of the I-V curve occur near the main resonance  $\lambda \approx 1$ ). These portions are stable, perhaps contrarily to physical intuition.

We also calculated the (linear) stability-instability behavior of all of the computed branches of solutions to (38).

#### IV. SPECIAL METHODS FOR QUADRATIC SYSTEMS OF DIFFERENTIAL EQUATIONS

The fractional linear scheme

$$u(t+h) = (-\hat{R}(h)[u(t)] + S(h))^{-1}(T(h)u(t) + v(h)) \quad (41)$$

was previously applied to the numerical solution of

$$\dot{x} = q(t, x)$$

where  $q$  is quadratic. It was shown [11] that convergent second-order accurate schemes of the above form exists for all quadratic systems and an explicit construction of such a scheme was given.

These results were extended to equations of the form

$$\dot{x} = (-R[x] + I)^{-1}(x \cdot x + Bx + c) \quad (42)$$

where  $R[x]x = 0$ . In particular, it was shown that i) a convergent fractional linear scheme converges to an equation of type (42); ii) every equation of type (42) can be solved numerically by a second-order accurate convergent fractional linear scheme.

A complete set of invariants was derived for all two-by-two systems of first-order quadratic differential equations, with respect to the six-parameter group of all affine transformations. These invariants provide a criterion for deciding to which affine equivalence class any given system belongs. Furthermore, all members of any one of these equivalence classes were shown to be equivalent to a single second-order equation in one dependent variable. Special cases of the latter define the set of all elliptic functions and other abelian integrals. A novel convergent second-order discretization of the above mentioned second-order equation was also proposed.

## V. CUMULATIVE LIST OF PUBLICATIONS

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